High-accuracy finite-difference time domain algorithm for the coupled wave equation

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Using a nonstandard (NS) finite difference model, we derived a high-accuracy finite-difference time domain algorithm to solve the coupled wave equation. The conventional NS-Yee algorithm can greatly reduce the error of the difference approximation and accurately solve the Maxwell's equations even for sub-wavelength whispering gallery modes, which are very sensitive to the scatterer model on the numerical grid. However, relative to the transverse magnetic mode, the error in the transverse electric mode is large because $\nabla\varepsilon$ (ε=permittivity) is not accurately represented [J. Opt. Soc. Am. B **27**, 631 (2010)]. In this paper, we derive a nonstandard finite-difference time domain algorithm to solve the coupled wave equation which accurately includes $\nabla\varepsilon$, and we demonstrate its higher accuracy and shorter computing time. © 2010 Optical Society of America

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1. INTRODUCTION

In nonconducting, dispersion-less, and linear isotropic media the Maxwell equations become

$$-\mu\partial_t\mathbf{H}=\nabla\times\mathbf{E}, \tag{1}$$

$$\varepsilon\partial_t\mathbf{E}=\nabla\times\mathbf{H}, \tag{2}$$

where $\partial_t=\partial/\partial t$, ε is the permittivity, μ is the permeability, $\mathbf{E}=(E_x,E_y,E_z)$ is the electric field, and $\mathbf{H}=(H_x,H_y,H_z)$ is the magnetic field. The nonstandard (NS)-Yee algorithm [1] can accurately solve the Maxwell equations even for sub-wavelength whispering gallery modes (WGMs).

WGMs are resonances in the interiors of highly symmetric structures such as infinite cylinders and spheres. WGMs strongly confine the light to the structure because the electromagnetic field outside the structure is weakly coupled to the inside. Thus the excitation is very slow and the error accumulates in the simulation. Sub-wavelength WGMs are especially sensitive to the scatterer model on the numerical grid [2].

In simulations of sub-wavelength WGMs, we found that the error of the NS-Yee algorithm is larger in the transverse electric (TE) mode ($\mathbf{E}$ perpendicular to media interfaces) than in the transverse magnetic (TM) mode ($\mathbf{E}$ parallel to media interfaces). We believe that this higher error arises because $\nabla\varepsilon$ is not accurately represented in the NS-Yee algorithm. In the TM mode, Gauss' law, $\nabla\cdot(\varepsilon\mathbf{E})=\mathbf{E}\cdot\nabla\varepsilon+\varepsilon\nabla\cdot\mathbf{E}=0$, gives

$$\mathbf{E}\cdot\nabla\varepsilon=\nabla\cdot\mathbf{E}=0, \tag{3}$$

because of $\mathbf{E}\perp\nabla\varepsilon$. Thus the Maxwell equations reduce to the homogeneous wave equation,

$$(\partial_t^2-v^2\nabla^2)\mathbf{E}=0, \tag{4}$$

where $v=1/\sqrt{\varepsilon\mu}$. The NS-Yee algorithm gives excellent results in the TM mode, because it is optimized to the homogeneous wave equation. In the TE mode, however, Eq. (3) is not satisfied because $\mathbf{E}\|\nabla\varepsilon\Rightarrow\nabla\cdot\mathbf{E}\neq0$, and we are left with the inhomogeneous coupled wave equation,

$$(\partial_t^2-v^2\nabla^2)\mathbf{E}=-v^2\nabla(\nabla\cdot\mathbf{E}). \tag{5}$$

At media interfaces, in the TE mode the NS-Yee algorithm does not accurately include $\nabla(\nabla\cdot\mathbf{E})$ because it is optimized to the homogeneous wave equation.

Other authors have considered a coupled wave equation approach [3,4], but found no particular advantage. In this paper, using a nonstandard finite-difference (NS-FD) model [5], we derive a high-accuracy nonstandard finite-difference time domain (NS-FDTD) algorithm to solve the coupled wave equation which accurately includes $\nabla\varepsilon$, and we demonstrate its high accuracy and greater computing speed.

For brevity and to avoid confusion, hereafter, by "FDTD" we mean the finite-difference time domain (FDTD) algorithm to solve the coupled wave equation. The Yee algorithm solves the Maxwell equations.

2. FDTD ALGORITHMS FOR COUPLED WAVE EQUATION

A. Standard FDTD Algorithm

The finite-difference (FD) approximation to a derivative is given by

$$\frac{df(x)}{dx} \simeq \frac{d_x f(x)}{h}, \tag{6}$$

where h is the grid spacing and d_x is the difference operator defined by $d_x f(x)=f(x+h/2)-f(x-h/2)$. For reasons that will soon be obvious we call Eq. (6) the standard finite-difference (S-FD) approximation. Analogously we define d_y and d_t.

In the TE mode the coupled wave equation can be expanded for the E_x component,

$$\partial_t^2 E_x = v^2(\partial_y^2 E_x - \partial_x \partial_y E_y). \tag{7}$$

Replacing the derivatives in Eq. (7) with the S-FD approximations, we obtain

$$d_t^2 E_x = \frac{v^2 \Delta t^2}{h^2}(d_y^2 E_x - d_x d_y E_y). \tag{8}$$

Expanding $d_t^2 E_x$ and solving for $E_x(x,y,t+\Delta t)$ yields the standard finite-difference time domain (S-FDTD) algorithm,

$$E_x^{t+\Delta t} = -E_x^{t-\Delta t} + 2E_x^t + \frac{v^2 \Delta t^2}{h^2}(d_y^2 E_x^t - d_x d_y E_y^t), \tag{9}$$

where for simplicity we write $E_x(x,y,t) \to E_x^t$. The E_y formulation is obtained by exchanging x and y in Eq. (9).

Each electric field component lies at a different position on the numerical grid so that central FD approximations can be used for the spatial derivatives. As shown in Fig. 1, our arrangements are

$$E_x^t \to E_x(x, y + h/2, t), \tag{10}$$

$$E_y^t \to E_y(x + h/2, y, t). \tag{11}$$

The scattered field formula also can be derived easily. The total electric field $\mathbf{E}$ can be decomposed into a sum of the incident field $\mathbf{E}^0$ and the scattered field $\mathbf{E}^s$. $\mathbf{E}^0$ satisfies the homogeneous wave equation (4). Using $v=v_0$ in Eq. (4) and subtracting from Eq. (5), we obtain the coupled wave equation for the scattered field,

$$(\partial_t^2 - v^2\nabla^2)\mathbf{E}^s = -\nabla(\nabla \cdot \mathbf{E}^s) + \mathbf{J}, \tag{12}$$

where $\mathbf{J}$ is the source term and is given by

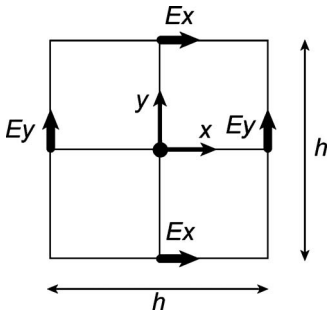

Fig. 1. Layout of the electric field on the numerical grid (h = grid spacing). $E_x(x,y+h/2)$ and $E_y(x+h/2,y)$ lie at different positions.

$$\mathbf{J} = \left(\frac{v^2}{v_0^2} - 1\right)\partial_t^2 \mathbf{E}^0. \tag{13}$$

The S-FDTD algorithm for the scattered field also can be derived in a similar way.

B. Nonstandard FDTD Algorithm

The error of the S-FD approximation is defined by $\epsilon^S f(x) = (h\partial_x - d_x)f(x)$ and $\epsilon^S \propto h^2$. One could try to reduce the error by using higher-order FD approximations, but this not only complicates the algorithm but also a higher-order difference equation may have unstable spurious solutions. Using what is called the NS-FD approximation [5], however, it is possible to greatly reduce the error of the FDTD algorithm without reducing the grid spacing or using higher order FD approximations.

In one dimension the NS-FD approximation has the form

$$\frac{df(x)}{dx} = \frac{d_x f(x)}{s(h)}, \tag{14}$$

where $s(h)$ is a correction function. It might seem that the choice $s(h)=d_x f(x)/f'(x)$ would make the approximation error vanish, but this choice is not always valid because the right side of Eq. (14) must converge to $f'(x)$ in the limit $h \to 0$. For a monochromatic wave e^{ikx} (k = wave number) an exact FD expression is obtained by putting $s(h) \to s(k,h)$, where

$$s(k,h) = \frac{2}{k}\sin\left(\frac{kh}{2}\right). \tag{15}$$

Analogously we find $\partial_t f(t) = d_t f(t)/s(\omega, \Delta t)$ for $f(t)=e^{\pm i\omega t}$ (ω = angular frequency).

In two or three dimensions, however, there is no exact NS-FD expression for the spatial derivatives because $s(\mathbf{k},h)$ depends on direction of the wave, $\mathbf{k}=(k_x,k_y)$. We found that the spatial error can be greatly reduced by using NS-FD approximations. In Eq. (7), there are two spatial derivatives: ∂_y^2 and $\partial_x \partial_y$. First we consider the S-FD approximations of ∂_y^2. The error is defined by

$$\epsilon_{yy}^S \varphi = (h^2 \partial_y^2 - d_y^2)\varphi, \tag{16}$$

where $\varphi = e^{i(k_x x + k_y y)}$ and $(k_x,k_y) = k(\cos\theta, \sin\theta)$. Expanding in a Taylor series, we find

$$\epsilon_{yy}^S = k^4 h^4\left(-\frac{\sin^2\theta}{12} + \frac{\sin^2(2\theta)}{48}\right) + k^6 h^6\left(\frac{\sin^2\theta}{360} - \frac{\sin^2(2\theta)(1+\sin^2\theta)}{1440}\right) + O(k^8 h^8), \tag{17}$$

where $O(k^8h^8)$ denotes terms of order h^8 or higher. We found a good NS-FD approximation by using $s_{yy}(k,h) = (2/k)\sin(kh/2)$. Putting $h \to s_{yy}(k,h)$ in Eq. (16), we obtain

$$\epsilon_{yy}^{NS} = k^4 h^4 \frac{\sin^2(2\theta)}{48} - k^6 h^6 \frac{\sin^2(2\theta)(1+\sin^2\theta)}{1440} + O(k^8 h^8). \tag{18}$$

Next we consider the S-FD approximation of $\partial_x\partial_y$. Similarly, the error is defined by

$$\epsilon_{xy}^{S}\varphi = (h^2\partial_x\partial_y - d_x d_y)\varphi. \tag{19}$$

Expanding in a Taylor series, we find

$$\epsilon_{xy}^{S} = -k^4h^4\frac{\sin(2\theta)}{48} + k^6h^6\left(\frac{\sin(2\theta)}{3840} + \frac{\sin^3(2\theta)}{11,520}\right) + O(k^8h^8). \tag{20}$$

We found a very good NS-FD approximation by using $s_{xy}(k,h)=\sqrt{(2h/k)\sin(kh/2)}$. Putting $h\to s_{xy}(k,h)$ in Eq. (19), we obtain

$$\epsilon_{xy}^{NS} = k^6h^6\frac{\sin^3(2\theta)}{11,520} + O(k^8h^8). \tag{21}$$

Replacing derivatives in Eq. (5) with the NS-FD approximations, we obtain a new NS-FDTD algorithm to solve the coupled wave equation,

$$E_x^{t+\Delta t} = -E_x^{t-\Delta t} + 2E_x^t + u_1 d_y^2 E_x^t - u_2 d_x d_y E_y^t, \tag{22}$$

where

$$u_1 = \frac{\sin^2(\omega\Delta t/2)}{\sin^2(kh/2)}, \tag{23}$$

$$u_2 = \frac{2\sin^2(\omega\Delta t/2)}{kh\sin(kh/2)}. \tag{24}$$

The E_y formulation is obtained by exchanging x and y in Eq. (22).

The NS scattered field formula can be derived in a similar way from Eq. (12). In three dimensions the NS-FD approximations also can be used for ∂_z^2, $\partial_x\partial_z$, $\partial_y\partial_z$.

3. NUMERICAL STABILITY

In homogeneous media, the numerical stability of the FDTD algorithm is the same as the Yee algorithm. Here we derive the stability conditions for inhomogeneous media. The S-FDTD and NS-FDTD algorithms can be cast into the generic form

$$\mathbf{E}_{n+1} = -\mathbf{E}_{n-1} + A\mathbf{E}_n, \tag{25}$$

where $\mathbf{E}^t\to\mathbf{E}_n$ for $t=n\Delta t$ (n=integer) and A is given by

$$A = \begin{pmatrix} 2+u_1d_y^2 & -u_2d_xd_y \\ -u_2d_xd_y & 2+u_1d_x^2 \end{pmatrix}. \tag{26}$$

In the S-FDTD algorithm $u_1=u_2=v^2\Delta t^2/h^2$, and in the NS-FDTD algorithm u_1 and u_2 are defined by Eqs. (23) and (24). Expanding Eq. (25), we find

$$\mathbf{E}_{n+1} = -P_n\mathbf{E}_0 + P_{n+1}\mathbf{E}_1, \tag{27}$$

where P_n and P_{n+1} are given by

$$\begin{pmatrix} P_n \\ P_{n+1} \end{pmatrix} = \underbrace{\begin{pmatrix} 0 & I \\ -I & A \end{pmatrix}}_{\mathbf{B}}{}^n \begin{pmatrix} 0 \\ I \end{pmatrix}, \tag{28}$$

where I is the identity matrix. If P_n does not diverge as $n\to\infty$, the algorithm is stable. Thus the stability condition is $|\Lambda|\le 1$, where Λ is the eigenvalue of the block matrix $\mathbf{B}$. To compute Λ, we solve

$$\left|\mathbf{B} - \Lambda\begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix}\right| = 0. \tag{29}$$

Defining $d_x\varphi=D_x\varphi$ (D_y is analogously defined), we evaluate the difference operators with respect to the monochromatic wave φ and obtain

$$D_x^2 = -4\sin^2(k_xh/2), \tag{30}$$

$$D_y^2 = -4\sin^2(k_yh/2), \tag{31}$$

$$D_xD_y = -4\sin(k_xh/2)\sin(k_yh/2), \tag{32}$$

and evaluate Λ with respect to φ. The most severe constraint is obtained by putting $D_x^2=D_y^2=D_xD_y=-4$,

$$\Lambda = \begin{pmatrix} 1-2u_+ \pm \sqrt{u_+(u_+-1)} \\ 1-2u_- \pm \sqrt{u_-(u_--1)} \end{pmatrix}, \tag{33}$$

where $u_\pm=u_1\pm u_2$. Using $|\Lambda|\le 1$, the stability condition of the S-FDTD algorithm becomes

$$\frac{v\Delta t}{h} \le \frac{1}{\sqrt{2}} \simeq 0.7071. \tag{34}$$

Using $\omega=vk$ and $k=2\pi/\lambda$, the stability condition of the NS-FDTD algorithm becomes

$$\frac{v\Delta t}{h} \le \frac{\alpha}{\pi}\arcsin\left(\frac{\sqrt{\pi}\sin(\pi/\alpha)}{\sqrt{\pi+\alpha\sin(\pi/\alpha)}}\right), \tag{35}$$

where $\alpha=\lambda/h$. Figure 2 shows $\max(v\Delta t/h)$ as a function of λ/h. The stability conditions of the S-FDTD and NS-FDTD algorithms become the same as $\lambda/h\to\infty$.

4. ALGORITHM VERIFICATION

A. Accuracy Comparison: S-FDTD versus NS-FDTD

For sub-wavelength Mie scattering (off-resonance) and WGM (on-resonance), we compared the S-FDTD and NS-FDTD algorithms to solve the coupled wave equation with Mie theory [6] and verified its accuracy. We calculate the scattering due to an infinite plane wave impinging upon a dielectric cylinder in the TE mode (Fig. 3). We choose the incident wave vector to be in the direction of the positive

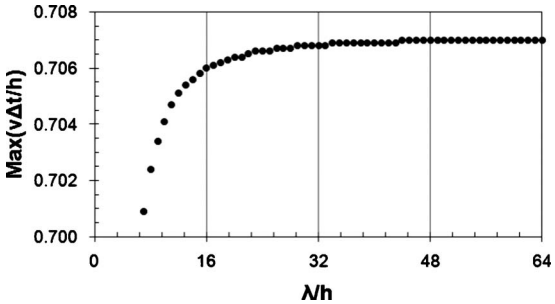

Fig. 2. Stability. Maximum allowed value of $v\Delta t/h$ for the NS-FDTD algorithm (λ=wavelength, h=grid spacing).

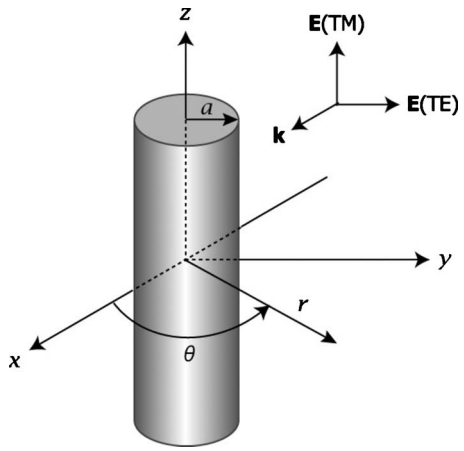

Fig. 3. Infinite plane wave impinging on an infinite dielectric cylinder (a=radius, k=wave vector). TM and TE polarizations are shown. Wave propagates along +x-axis.

x-axis and the incident electric field to be polarized in the y-direction. Since the scattered field intensity $|E_x^s|^2$ is relatively small, we examine $|E_y^s|^2$.

We terminate the computational domain with Higdon's absorbing boundary condition [7]. We modeled the scatterer on the grid using the TE fuzzy model [2]. Example parameters used for off- and on-resonance calculations are listed in Table 1.

In Figs. 4 and 5(a)–5(c) we visualize the converged $|E_y^s|^2$ distributions (at 500 time steps off-resonance; 100,000 time steps on-resonance). In Figs. 4 and 5(d) we plot $|E_y^s|^2$ on a circular contour of radius $1.1a$ around the cylinder center (a=cylinder radius). As shown in Figs. 4 and 5, the NS-FDTD algorithm is much more accurate than the S-FDTD one. The accuracy for the WGM is slightly lower than for off-resonance, because during the long excitation time errors accumulate and the TE fuzzy model does not accurately capture all aspects of the scatterer shape.

B. Accuracy: Yee versus NS-FDTD

For the sub-wavelength WGM, we compared the accuracy of the Yee algorithms (to solve the Maxwell equations) with the NS-FDTD algorithm (to solve the coupled wave equation). We calculated the root-mean-square (RMS) error of the converged scattered intensity relative to Mie theory in Fig. 6. The simulation parameters are the same as in Table 1 (on-resonance) except for the grid size.

As seen in Fig. 6, on a coarse grid (small value of λ/h), the NS-Yee algorithm is more accurate than the NS-FDTD one since the NS-Yee error in a uniform medium is proportional to k^6h^6 and the NS-FDTD error is proportional to k^4h^4. On a finer grid (large value of λ/h), however, the NS-FDTD algorithm is somewhat more accurate because here the dominant source of error is the error of the scatterer grid model. On the other hand, in the NS-FDTD algorithm, the error of the scatterer model error on the numerical grid is smaller.

Table 1. Computational Parameters in the Simulation of the S-FDTD Algorithm versus the NS-FDTD One

Off-Resonance	
Grid size	80 nm × 80 nm
Wavelength	640 nm
Cylinder radius	640 nm
Computation space	5120 nm × 5120 nm
Refractive index	1.6
On-Resonance (WGM)	
Grid size	10 nm × 10 nm
Wavelength	640 nm
Cylinder radius	320 nm
Computation space	1280 nm × 1280 nm
Refractive index	2.683

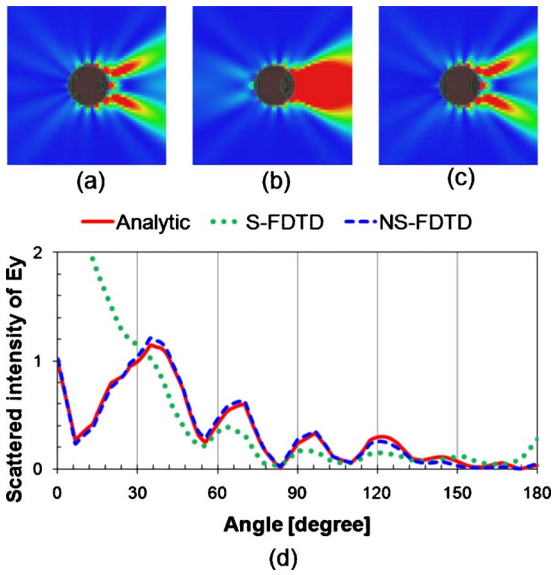

Fig. 4. (Color online) Off-resonance FDTD calculation of $|E_y^s|^2$. The intensity distributions are visualized. (a) Analytical solution. (b) S-FDTD calculation. (c) NS-FDTD calculation. (d) Angular intensity distributions.

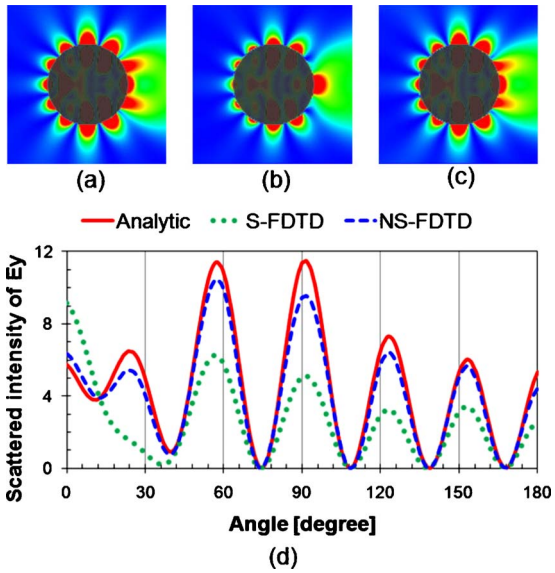

Fig. 5. (Color online) WGM (on-resonance) FDTD calculation of $|E_y^s|^2$. The intensity distributions are visualized. (a) Analytical solution. (b) S-FDTD calculation. (c) NS-FDTD calculation. (d) Angular intensity distributions.

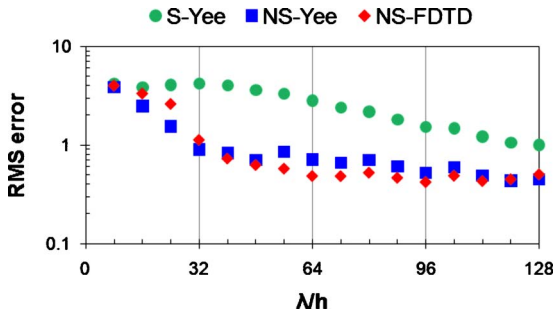

Fig. 6. (Color online) RMS error in the $|E_y^s|^2$ angular distribution as a function of grid fineness, for the sub-wavelength WGM. The converged time is defined by $10,000\times(\lambda/h)/64$.

C. Computational Cost: Yee versus NS-FDTD

We compared the storage cost and computing time of the Yee algorithms with the NS-FDTD algorithm. The storage cost of our coupled wave equation approach is the same as the Yee algorithms, because the coupled wave equation includes ∂_t^2 operator which requires $\mathbf{E}^t$ and $\mathbf{E}^{t-\Delta t}$ to calculate $\mathbf{E}^{t+\Delta t}$, whereas the Maxwell equations compute both $\mathbf{E}$ and $\mathbf{H}$.

Since only $\mathbf{E}$ is computed in the coupled wave equation, the NS-FDTD algorithm can reduce the computing time relative to Yee algorithms; however, both Yee and NS-FDTD algorithms need the same number of time steps to converge. In Fig. 7, we plotted the computing time for 1000 steps as a function of the grid fineness. As seen in Fig. 7, the NS-FDTD algorithm is about twice as fast as the Yee algorithms. Note that the magnetic field can be computed from the Maxwell equations easily using the electric field.

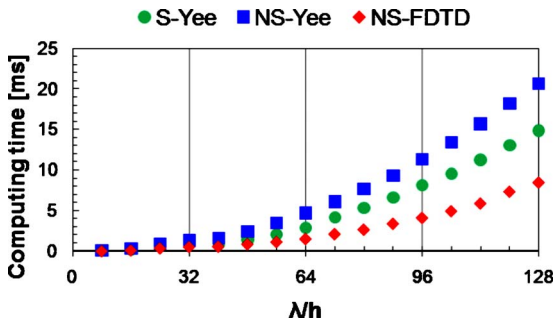

Fig. 7. (Color online) Computing time for 1000 steps as a function of grid fineness [using Intel(R) Core(TM) 2 Duo Processor 2.33 GHz, DDR2–800 SDRAM].

5. CONCLUSION AND DISCUSSION

We developed a nonstandard finite difference time domain (NS-FDTD) algorithm to accurately solve the coupled wave equation. This NS-FDTD algorithm theoretically takes into account $\nabla\varepsilon$ better than the conventional NS-Yee algorithm.

We demonstrated that the NS-FDTD algorithm is much more accurate than the conventional standard finite difference time domain (S-FDTD) algorithm and can accurately solve the sub-wavelength whispering gallery mode (WGM). The NS-FDTD algorithm is the same or more accurate than the NS-Yee one. We also demonstrated that our algorithm runs about twice as fast as the Yee algorithms. We are now extending our work to three dimensions and dispersive materials.

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